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Self consistent microscopic theory of frictional ratchet in a nonequilibrium environment

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Abstract . A system-reservoir microscopic model, where the associated reservoir is modulated by the external random force, is proposed to study the transport of an overdamped Brownian particle in a frictional ratchet system with an underlying periodic potential in presence of external Gaussian noise fluctuation We then derived the analytical expression for the average velocity and study the dependence of the various system parameters and the nonequilibrium behavior of the heat bath on the transport properties of the Brownian particle. We observe that only bath modulation though it breaks the fluctuation-dissipation relation, will not produce any net current in absence of external modulation.

Keywords Frictional ratchet, system-reservoir model, non-linear multiplicative Langevin equation, overdamped Brownian particle.

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1. Introduction

Thermal diffusion in a periodic potential has a prominent role in various systems such as Josephson's junction [1], systems for diffusion in crystal surfaces [2], noisy limit cycle oscillators [3] *etc.* There has been a renewed interest in recent times in the study of transport properties of Brownian particles moving in a periodic potential [4] with special emphasis on coherent transport and giant diffusion [5]. These studies have been motivated in part by the attempt to understand the mechanism of movement of protein motors in biological system [6]. Several physical models have been proposed to understand the transport phenomenon in such systems, such as vibrational ratchet [7], rocking ratchets [8], flashing ratchets [5], diffusion ratchets [9, 10], correlation ratchets [11] *etc.* Such

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ratchet models have a wide range of applications in biology and nanoscopic systems [12], because of its extraordinary success in exploring experimental observations on biochemical molecular motors, active in muscle contraction [13], observation on directed transport in photovoltaic and photoreflective materials [14] *etc* In all the above models the potential is taken to be asymmetric in space One can also obtain a unidirectional current in the presence of spatially symmetric potential For such nonequilibrium systems one requires time asymmetric random force [15] or space dependent diffusion [16-18] Space dependent diffusion coefficient may arise either due to space dependent temperature or space dependent friction coefficient [18] Frictional inhomogeneities are common in superlattice structure, semiconductors or motion in porous media Particles moving close to a surface experience space dependent friction [19] Molecular motor proteins moving along the periodic structures of microtubles experience a space dependent friction [20] Based on a system-reservoir nonlinear coupling model very recently Ray *et al* [21] have presented a microscopic approach to quantum state-dependent diffusion and multiplicative noise

To the best of our knowledge in almost all the works relating transport properties of a ratchet system, the Langevin equation is either written phenomenologically or have been constructed from a microscopic Hamiltonian system-reservoir model where the associated bath is in thermal equilibrium In the present paper we consider a system-reservoir model where the system and reservoir both are modulated by external noise and the system is nonlinearly coupled with the heat bath thereby resulting in a nonlinear multiplicative Langevin equation with space dependent diffusion However, when the reservoir is mudulated by an external noise, it is likely that it induces fluctuations in the polarization of the reservoir [22] due to the external noise and one may expect that the nonequilibrium situation created by modulating the bath may induce an asymmetry in the effective potential, thereby generating a directed transport A direct driving usually breaks the fluctuation-dissipation relation and generates a biased directed motion [23] of the system (where the associated bath is in thermal equilibrium) Here we are interested in a situation where the associated bath is modulated by external random force to study the directed transport of a frictional ratchet system The problem of particle motion in inhomogeneous media in presence of an external noise becomes equivalent to the problem in a space dependent temperature, generating unidirectional current This follows as a corollary to Landauer's blow-torch effect [24] It has been shown earlier by us [22] that the bath modulation by an external force creates an environment with an effective temperature that depends on the coupling constant and strength of the external noise

A number of different situations depicting the modulation of the bath may be physically relevant Though the dynamics of a Brownian particle in a uniform solvent is well known, it is not very clear when the response of the solvent will be time dependent, as in a liquid crystal, or in diffusion and reaction in supercritical liquids and growth in living polymerization [25] Also space dependent friction is realized from the presence of a stochastic potential in the Langevin equation [26] As another example, we may consider a simple unimolecular conversion from $A \rightarrow B$, say, an isomerization reaction The reaction can be carried out in a photochemically active solvent Since the fluctuation in the light intensity results in fluctuation in the polarization of the solvent molecules, the effective reaction field around the reactant system gets modified In the present work, we address the problem of Langevin equation with multiplicative noise and state dependent diffusion for a thermodynamically open system and we explore the nature of nonlinear coupling and its consequences, specially the possibility of observing directed transport in a periodic potential as a consequence of state dependent diffusion, where the associated bath is modulated by external noise

The organization of the paper is as follows In Section 2 starting from a Hamiltonian picture of a system non-linearly coupled with the harmonic reservoir which is modulated by a noise, we have derived the generalized Langevin equation with an effective multiplicative noise $\eta(t)$ and an additive noise The statistical properties of the multiplicative noise have been explored In Section 3 we have constructed the Fokker-Planck equation, corresponding to the Langevin equation, in configuration space after properly eliminating the fast variables and have calculated the net current in a sinusoidal potential The paper has been concluded in Section 4

2. The model : heat bath modulated by external noise

We consider a classical particle of unit mass is coupled to a heat bath consisting of a set of N number of mass-weighted harmonic oscillators with frequency $\{\omega_j\}$ Both the system and the heat bath is externally driven by a Gaussian random force $\epsilon(t)$ which has arbitrary decaying correlation time The total Hamiltonian of such a composite system can be written as

$$H = \frac{p^2}{2} + V(q) + \sum_{j=1}^{N} \left\{ \frac{p_j^2}{2} + \frac{1}{2}\omega_j^2 \left(x_j - c_j f(q)\right)^2 \right\} + \sum_{j=1}^{N} k_j x_j \epsilon(t) - \alpha q \epsilon(t) \quad (2\,1)$$

In the above equation q and p are the coordinate and the momentum of the system particle, respectively, and $V(q)$ is the potential energy of the system $\{x_j, p_j\}$ are the variables for the jth oscillator The system particle is coupled to the bath oscillators nonlinearly through the general coupling terms $c_j \omega_j f(q)$ where c_j is the coupling strength for the system-bath interaction The interaction between the heat bath and the external noise is represented by the fourth term, where k_j denotes the strength of interaction The last term is the direct driving term with coupling constant α We consider $\epsilon(t)$ to be a stationary Gaussian noise with zero mean and arbitrary decaying correlation function

$$\langle \epsilon(t) \rangle_e = 0, \quad \langle \epsilon(t)\epsilon(t') \rangle_e = 2D\Psi(t-t') \quad (2\,2)$$

where D is the strength of external noise, $\Psi(t-t')$ is the kernel of the external noise and $\langle\ \rangle_e$ implies averaging over each realization of $\epsilon(t)$

Eliminating the bath degrees of freedom in the usual way [27] we get the following Langevin equation

$$\dot{q} = p$$

$$\dot{p} = -V'(q) - f'(q(t))\int_0^t dt'\gamma(t-t')\, f'(q(t'))p(t') + f'(q(t))F(t) + f'(q(t))\pi(t) + \alpha\varepsilon(t) \quad (2\ 3)$$

where the memory kernel $\gamma(t)$ and the Langevin force term $F(t)$ are given respectively by

$$\gamma(t) = \sum_{j=1}^{N} c_j^2\omega_j^2 \cos\omega_j t \quad (2.4)$$

and

$$F(t) = \sum_{j=1}^{N} c_j^2\omega_j^2 \left[\left\{x_j(0) - c_j f(q(0))\right\}\cos\omega_j t + \frac{p_j(0)}{\omega_j}\sin\omega_j t\right. \quad (2.5)$$

$\pi(t)$ is the fluctuating force generated due to the external stochastic forcing of the bath by $\varepsilon(t)$ and is given as

$$\pi(t) = -\int_0^t dt'\varphi(t-t')\,\varepsilon(t') \quad (2.6)$$

where

$$\varphi(t) = \sum_{j=1}^{N} c_j k_j \omega_j \sin\omega_j t \quad (2.7)$$

The form of eq. (2.3) reveals that the system is driven by two fluctuating forces $F(t)$ and $\varepsilon(t)$. $\pi(t)$ is a dressed noise originated due to bath modulation by external noise $\varepsilon(t)$. $F(t)$ and $\pi(t)$ appears multiplicatively while $\varepsilon(t)$ appears additively. To define the statistical properties of $F(t)$, we assume that the initial distribution in one in which the bath is equilibrated at $t = 0$ in the presence of system but in the absence of the external noise $\varepsilon(t)$ such that

$$\langle F(t)\rangle = 0 \quad \text{and} \quad \langle F(t)F(t')\rangle = k_B T_\gamma(t-t') \quad (2.8)$$

where k_B is the Boltzmann constant and T is the equilibrium temperature. <...> implies the usual average over the initial distribution which is assumed to be a canonical distribution of Gaussian form, given by

$$\mathcal{P} = \mathcal{N} \exp\left\{ -\frac{p_j^2(0) + \omega_j^2\left(x_j(0) - c_j f(q(0))\right)^2}{2k_B T} \right\}$$

where $\mathcal{N}$ is the normalization constant Now at $t = 0_+$, the external noise agencies are switched on to modulate the bath and to drive the system by $\varepsilon(t)$ The dynamics of the system is then governed by eq (2 3), where apart from the internal noise $F(t)$ and external noise $\varepsilon(t)$, another fluctuating force $\pi(t)$ appears which depends on the external noise $\varepsilon(t)$ and is dressed by the function $\varphi(t)$ defined in eq (2 7) We can define an effective Gaussian noise $\eta(t) = F(t) + \pi(t)$ the statistical properties of which can be summarized by

$$\langle\langle \eta(t) \rangle\rangle = 0$$

$$\langle\langle \eta(t)\eta(t') \rangle\rangle = k_B T_\gamma(t - t') + 2D\int_0^t dt'' \int_0^t dt''' \times \varphi(t - t'')\varphi(t' - t''')\Psi(t'' - t''')$$

$$= G(t - t') \quad (say) \tag{2 9}$$

In eq (2 9) << >> means we have taken two averages, averages over initial distribution of bath variables and averages over each realization of $\varepsilon(t)$, independently While deriving eq (2 9) we have made the assumption $\langle\langle \eta(t)\eta(t') \rangle\rangle - G(t - t')$ which can not be proved unless the structure of $\varphi(t)$ is explicitly given As we shall see that it is a valid assumption for a particular choice of coupling coefficients $c(\omega)$ and $k(\omega)$ and for stationary external noise processes It should be realized that the above eq (2 9) is not a fluctuation-dissipation relation due to the appearance of the external noise intensity, rather it serves as a thermodynamic consistency relation

To obtain a finite result in the continuum limit, *i e*, for $N \to \infty$, the coupling function $c_i = c(\omega)$ and $k_i = k(\omega)$ are chosen as $c(\omega) = c_0 / (\omega\sqrt{\tau_c})$ and $k(\omega) = k_0 \omega \sqrt{\tau_c}$ Consequently $\gamma(t)$ and $\varphi(t)$ reduces to

$$\gamma(t) = \frac{c_0^2}{\tau_c} \int d\omega\, \mathcal{D}(\omega) \cos \omega t \tag{2 10}$$

and

$$\varphi(t) = c_0 k_0 \int d\omega\, \mathcal{D}(\omega)\omega \sin \omega t \tag{2 11}$$

where c_0 and k_0 are constants and τ_c is the correlation time of the bath For $\tau_c \to 0$ we obtain a δ-correlated noise process $1/\tau_c$ is characterized as the cutoff frequency of the reservoir oscillators $\mathcal{D}(\omega)$ is the density of modes of the heat bath which is assumed to be Lorentzian

$$\mathcal{D}(\omega) = \frac{2}{\pi\tau_c\left(\omega^2 + \tau_c^{-2}\right)} \tag{2 12}$$

The above assumption resembles broadly the behavior of the hydrodynamical modes in a macroscopic systems [28] With these forms of $\mathcal{D}(\omega)$, $c(\omega)$ and $k(\omega)$ we have the expression for $\varphi(t)$ and $\gamma(t)$ as

$$\gamma(t) = \frac{c_0^2}{\tau_c} \exp\left(-t/\tau_c\right), \tag{2 13a}$$

$$\varphi(t) = \frac{c_0 k_0}{\tau_c} \exp\left(-t/\tau_c\right) \tag{2 13b}$$

In passing we make the following two comments Though eq (2 9) is not a fluctuation dissipation relation, eq (2 6) resembles the familiar linear relation between the polarization and the external field Here $\pi(t)$ and $\varepsilon(t)$ play the role of former and latter, respectively Thus $\varphi(t)$ can be interpreted as a response function of the reservoir due to external noise $\varepsilon(t)$ It is also clear from the structure of $\varphi(t)$ and $\gamma(t)$ that

$$\frac{d\gamma(t)}{dt} = -\frac{c_0}{k_0}\frac{1}{\tau_c}\varphi(t) \tag{2 14}$$

The above relation is independent of $\mathcal{D}(\omega)$ and represents how the dissipative kernel $\gamma(t)$ depends on the response function $\varphi(t)$ of the medium due to the external noise $\varepsilon(t)$ Such an equation for the open system can be anticipated in view of the fact that both the dissipation and response functions crucially depend on the properties of the reservoir If we assume that $\varepsilon(t)$ is a δ-correlated noise, *i e*, $\left\langle \varepsilon(t)\,\varepsilon(t')\right\rangle_e = 2D\delta(t - t')$ then the correlation function of $\pi(t)$ is given by

$$\left\langle \pi(t)\pi(t')\right\rangle_e = \frac{Dc_0^2k_0^2}{\tau_c} \exp\left(-|t - t'|/\tau_c\right) \tag{2 15}$$

where we have neglected the transient terms $(t, t' > \tau_c)$ This equation shows how the heat bath dresses the external noise Though the external noise is a δ-correlated noise the system encounters it as an exponentially correlated noise with the same correlation time of the internal noise but with an intensity depending on the coupling k_0 and the external noise strength D On the other hand, if the external noise is an Ornstein-Uhlenbeck process with $\langle \epsilon(t)\,\epsilon(t')\rangle_e = D/\tau' \exp(-|t-t'|/\tau')$, the correlation function of $\pi(t)$ is found to be

$$\langle \pi(t)\pi(t')\rangle_e = \frac{D c_0^2 k_0^2}{(\tau'/\tau_c)^2 - 1}\frac{\tau'}{\tau_c}\left\{\frac{1}{\tau_c}\exp\left(-\frac{|t-t'|}{\tau'}\right) - \frac{1}{\tau'}\exp\left(-\frac{|t-t'|}{\tau_c}\right)\right\} \tag{2.16}$$

where we have neglected the transient terms The dressed external noise $\pi(t)$ now has a more complicated correlation function with two correlation times τ_c and τ' If the external noise-correlation time be much larger than the internal noise-correlation time i e $\tau' >> \tau_c$, which is more realistic then the dressed noise is dominated by the external noise and we have

$$\langle \pi(t)\,\pi(t')\rangle_e = \frac{D c_0^2 k_0^2}{\tau'}\exp\left(-\frac{|t-t'|}{\tau'}\right) \tag{2.17}$$

On the other hand, when the external noise correlation time is smaller than the internal one we recover (2 15)

With such an effective noise $\eta(t)$, the Langevin eq (2 3) can be written as

$$\dot q = p$$

$$\dot p = -V'(q) - f'(q(t))\int_0^t dt'\gamma(t-t')\,f'(q(t'))p(t') + f'(q(t))\eta(t) + \omega(t) \tag{2.18}$$

where the statistical property of $\eta(t)$ is given from eq (2 9)

3. Fokker-Planck equation and phase induced current

For Markovian internal dissipation and δ-correlated external noise $\epsilon(t)$, eq (2 18) reduces to

$$\dot q = p$$

$$\dot p = -V'(q) - \Gamma(q)p(t) + \sqrt{(k_B T + D_e k_0^2)\Gamma(q)}\,\beta(t) + \zeta(t) \tag{3.1}$$

where the state dependent dissipation constant $\Gamma(q)$ is given by

$$\Gamma(q) = \gamma\,[f'(q)]^2\ , \qquad \gamma = c_0^2$$

and $\beta(t)$ and $\xi(t)$ are two Gaussian δ-correlated noise with zero mean and

$$\langle\langle \beta(t)\beta(t')\rangle\rangle = 2\delta(t-t'), \tag{3.2a}$$

$$\langle\langle \xi(t)\xi(t')\rangle\rangle = 2B\delta(t-t'), \tag{3.2b}$$

where $B = D_e\alpha^2$ is the strength of the noise $\xi(t)$

On time scale larger than the inverse-friction coefficient, Γ^{-1} one can in most practical cases consider the overdamped limit of the Langevin equation This in turn corresponds to the adiabatic elimination of the fast variable, velocity, from the equation of motion for a homogeneous system But for the case of inhomogeneous system the above method does not work Sancho *et al* [29] has given a proper method for the elimination of fast variables The corresponding overdamped version of the above Langevin eq (3 1) then becomes

$$q = -\frac{V'(q)}{\Gamma(q)} - \frac{(k_B T + D_e k_0^2)\Gamma'(q)}{2[f'(q)]^2} + \sqrt{\frac{k_B T + D_e k_0^2}{\Gamma(q)}}\beta(t) + \frac{\xi(t)}{\Gamma(q)} \tag{3.3}$$

Using van Kampen's Lemma [30] and Novikov's theorem [31] the Fokker-Planck equation corresponding to eq (3 3) is then given by

$$\frac{\partial P(q,t)}{\partial t} = \frac{\partial}{\partial q}\left[\left\{\frac{V'(q)}{\Gamma(q)} - \frac{D\Gamma'(q)}{\Gamma^3(q)}\right\}P(q,t) + \left\{\frac{k_B T + D_e k_0^2}{\Gamma(q)} - \frac{B}{\Gamma^2(q)}\right\}\frac{\partial P(q,t)}{\partial q}\right] \tag{3.4}$$

For a periodic potential $V(q)$ and for the periodic coupling function $f(q)$ with periodicity 2π, a finite probability current is obtained and following Risken we get the expression for the average velocity as [4]

$$\langle v\rangle = 2\pi \frac{1-\exp(-\Delta)}{\int_0^{2\pi} dy \exp[-\phi(y)] \int_y^{y+2\pi} dx \frac{\exp[\phi(x)]}{A(x)}} \tag{3.5}$$

In eq (3 5) $\phi(q)$ is the generalized effective potential and is given by

$$\phi(q) = \int_0^q dq' \frac{V'(q')\Gamma^2(q') - B\Gamma'(q')}{\Gamma(q')\left[\{k_B T + D_e k_0^2\}\Gamma(q') + B\right]} \tag{3.6}$$

and $A(q)$ is the effective space dependent diffusion co-efficient and is given by

$$A(q) = \frac{\left\{\left\{k_B T + D_e k_0^2\right\} \Gamma(q) + B\right\}}{\Gamma^2(q)} \tag{3.7}$$

and

$$\Delta = \phi(q) - \phi(q + 2\pi) \tag{3.8}$$

is the effective slope of the generalized potential $\phi(q)$. The sign of Δ determines the direction of current <v>. In terms of periodic coupling function $f(q)$ and coupling constants $c_0^2(\gamma)$, k_0^2 and α, $\phi(q)$ and $A(q)$ can be expressed as

$$\phi(q) = \int_0^q dq' \frac{\gamma V'(q')\left[f^2(q')\right]^4 - 2D_e \alpha^2 f'(q') f''(q')}{\left[f'(q')\right]^2\left[\gamma\left(k_B T + D_e k_0^2\right)\left[f'(q')\right]^2 + D_e \alpha^2\right]} \tag{3.9}$$

and

$$A(q) = \frac{\gamma\left[f'(q)\right]^2 \left(k_B T + D_e k_0^2\right) + D_e \alpha^2}{\gamma^2\left[f'(q)\right]^4} \tag{3.10}$$

From the condition of periodicity of potential it is clear that for the periodic potential and the periodic derivative of the coupling function with same periodicity the slope Δ vanishes and consequently there will be no current. Thus there is no occurrence of current for a periodic potential and periodic derivative of coupling function with same periodicity and hence there is no violation of second law of thermodynamics. The thermodynamic consistency based on symmetry consideration ensures the validity of our present model. To continue, we consider the periodic potential $V(q) = V_0 \sin q$ which has the period 2π in which the Brownian particle is moving. The periodic coupling function $f(q)$ is given as $f(q) = q + \lambda\cos(q - \theta)$ so that $f'(q) = 1 - \lambda\sin(q - \theta)$, where λ is a modulation parameter and $0 < \lambda < 1$. The phase difference θ between potential $V(q)$ and $f(q)$ brings in the intrinsic asymmetry in the dynamics of the system.

We have studied the average velocity <v> as a function of different parameters. For various values of λ we have plotted <v> as a function of phase difference θ, in Figure 1 over a period π and in Figure 2 we have studied the average velocity <v> as a function of phase difference θ for various values α. In both the cases we obtained a periodic structure of current which vanishes for $\lambda = 0$ and $\alpha = 0$. $\lambda = 0$ implies the linear system-reservoir coupling and in such a case external driving by a δ-correlated noise even in the presence of bath modulation does not produce any current. On the other hand, <v> = 0 for α = 0 implies that only bath modulation by a white noise will not produce any directional motion. In a recent work [32] we have studied the effect of bath modulation by a colored noise and observed that the finite correlation time of the noise by

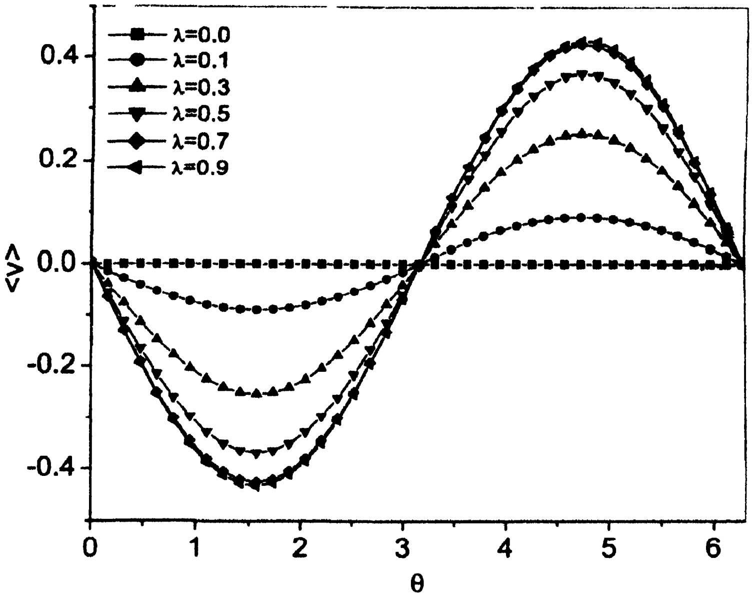

Figure 1. Variation of average velocity, <v>, with phase difference, θ, for various modulation parameter λ for the parameter set k_BT = 0.1, D_e = 0.36, k_0^2 = 1.0, α = 4.0, γ = 1.0 and V_0 = 1.0

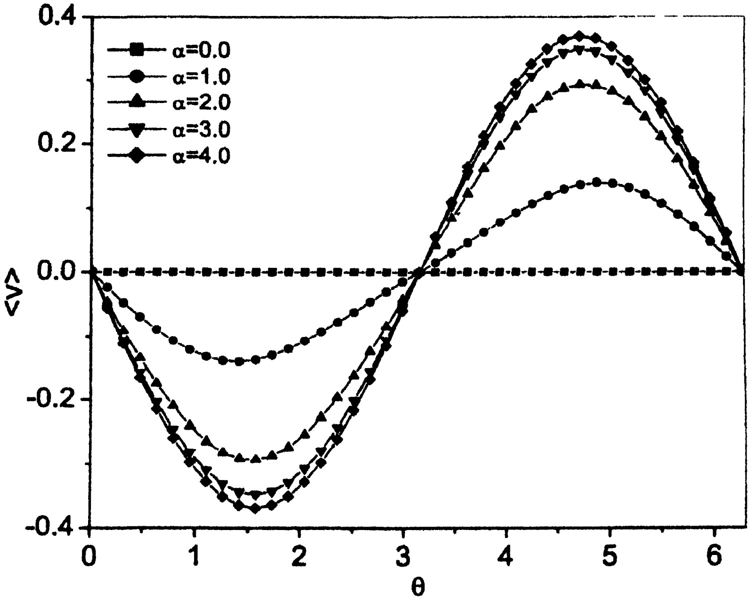

Figure 2. Variation of average velocity, <v>, with phase difference, θ, for various α for the parameter set k_BT = 0.1, D_e = 0.36, k_0^2 = 1.0, λ = 0.5, γ = 1.0 and V_0 = 1.0

which the bath is modulated can create unidirectional motion even for $\alpha = 0$ It is interesting to observe from Figure 1 and Figure 2 that i) for $\theta \neq 0$ $n\pi$ where $n = \pm 1$ $\pi 2$ the phase difference θ induces a current and ii) increases in λ or α results in increase in current In Figure 3 we have plotted current as a function of external noise

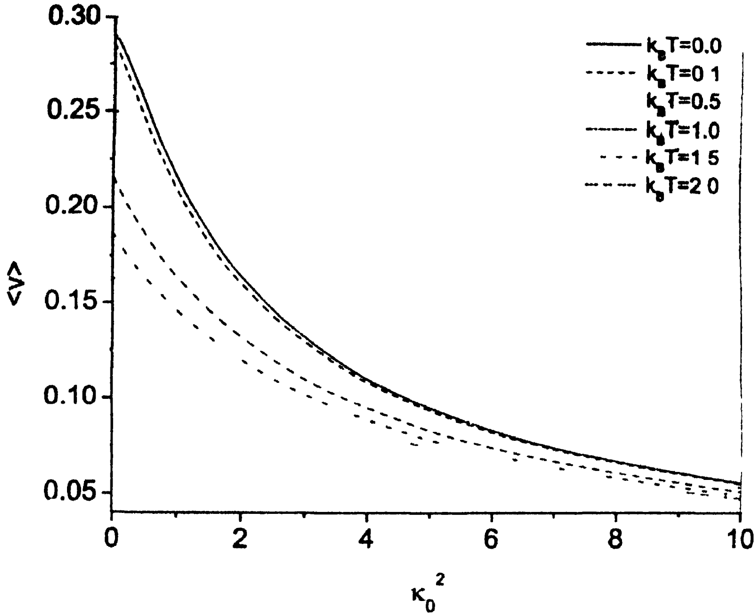

Figure 3 Variation of average velocity <v> with coupling constant k_0^2 for various temperature k_BT for the parameter set $\alpha = 0\ 1$ $\theta = 1\ 5\pi$ $D_e = 1\ 0$ $\gamma = 1\ 0$ $\lambda = 0\ 5$ and $V_0 = 1\ 0$

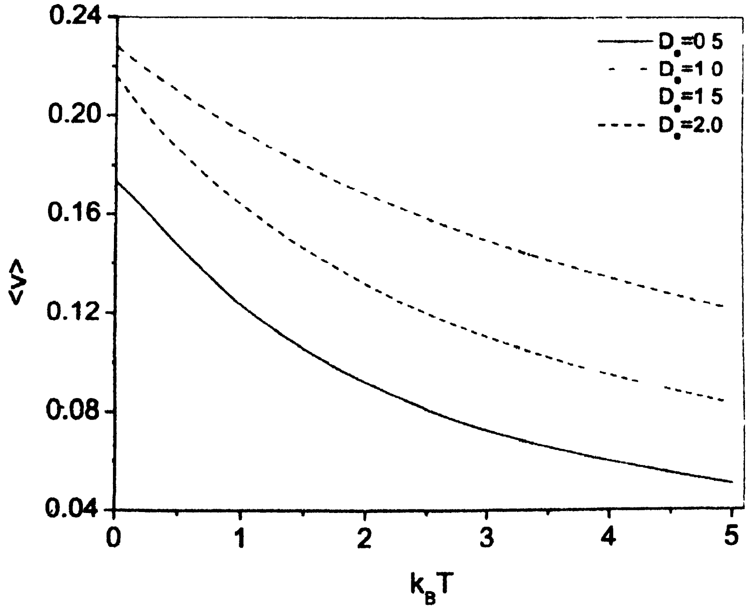

Figure 4 Variation of average velocity <v>, with temperature k_BT for various external noise strength D_e for the parameter set $\alpha = 0\ 1$ $\theta = 1\ 5\pi$ $k_0^2 = 1\ 0$ $\gamma = 1\ 0$ $\lambda = 0\ 5$ and $V_0 = 1\ 0$

coupling k_0^2 and observe that even for a zero temperature the external driving induces a finite current. For a particular temperature, increase in coupling k_0^2 results in the decrease in current nearly exponentially and for high k_0^2 the current becomes insensitive to k_0^2. It has been shown [22] that the bath modulation by an external Gaussian noise increases the effective temperature depending upon k_0^2. As observed in Figure 4, the fact that increase in temperature decreases current reflects our previous observation of Figure 3. In Figure 5 where we have plotted current as a function of α for particular D_e, we observe that the current vanishes for $\alpha = 0$. For any value of α, the current vanishes for the noise strength $D_e = 0$ (which reflects nothing but the thermodynamic consistency of our model). For $D_e \neq 0$, current increases rapidly with increase of α and for a large value of α it saturates.

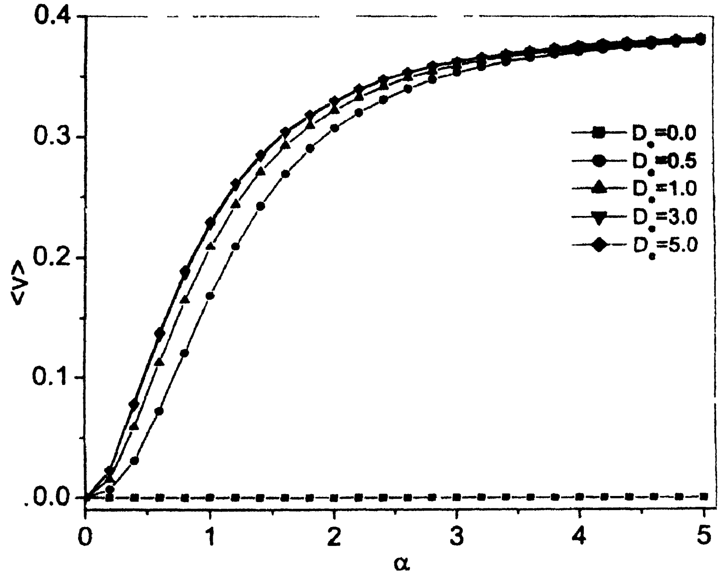

Figure 5. Variation of average velocity $<v>$ with α for various external noise strength D_e for the parameter set $k_BT = 0.1$, $\alpha = 1.5\pi$, $k_0^2 = 1.0$, $\gamma = 1.0$, $\lambda = 1.0$ and $V_0 = 1.0$.

4. Conclusion

A system-reservoir model, where the reservoir is modulated externally by a Gaussian noise, has been proposed to study the transport of an overdamped Brownian particle in a frictional ratchet system with an underlying sinusoidal potential in the presence of external Gaussian white noise fluctuations. The observation is that frictional inhomogeneities along with external fluctuations leads to the noise induced current or transport. The transport is associated with an effective potential and an effective space dependent diffusion coefficient. The effective potential exhibits a tilt as a function of system parameters, external coupling constant k_0 and noise strength D_e. An analytical measure of this tilt Δ has been derived and consequently we derived the expression of average velocity, i.e., the current. The thermodynamic consistency of our microscopic model has been checked. We then have studied the dependence of the current on various system parameters to show that in the absence of external fluctuation only bath modulation will not create any current, though the bath modulation breaks the fluctuation-dissipation relation The current will decrease with the increase of k_0 which reflects the fact that bath modulation increases the effective temperature of the bath

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